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Title:	Investigation of the impact of size effects and confined plasticity on stacking fault widths using 3D phase field dislocation dynamics (PFDD) simulations (U)
Author(s):	Abigail Hunter Irene Beyerlein Timothy Germann Marisol Koslowski
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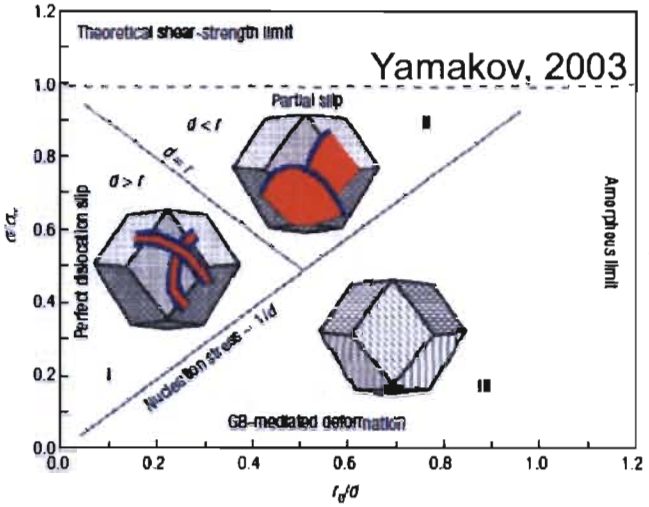
Investigation of the impact of size effects and confined plasticity on stacking fault widths using 3D phase field dislocation dynamics (PFDD) simulations

Abigail Hunter*, Irene Beyerlein, Tim Germann
Los Alamos National Laboratory

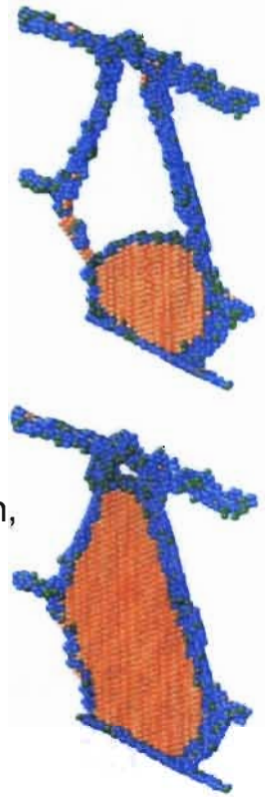
Marisol Koslowski
Purdue University

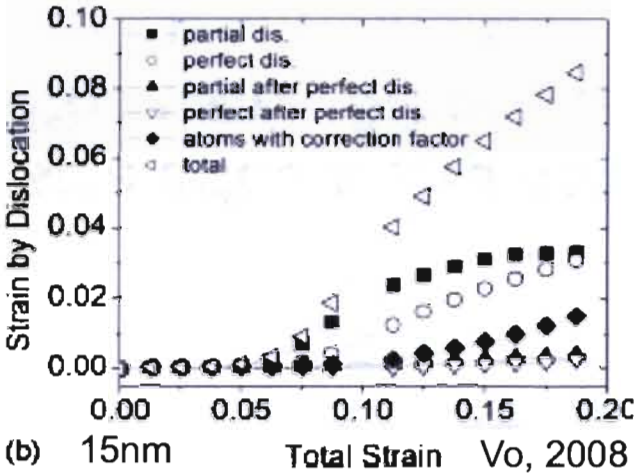
Nanocrystalline fcc Materials

- Transition in deformation mechanism in fcc metals as grain size decreases to the nano-scale (gs<100nm)
  - Dislocation-based ⟶ Grain boundary sliding (gs<10nm)
  - Length–scale competition between grain size and stacking fault width.
- At grain sizes of ~30-50nm, plastic deformation is primarily driven by the nucleation, interaction, and motion of partial dislocations.



Van Swygenhoven, 1999





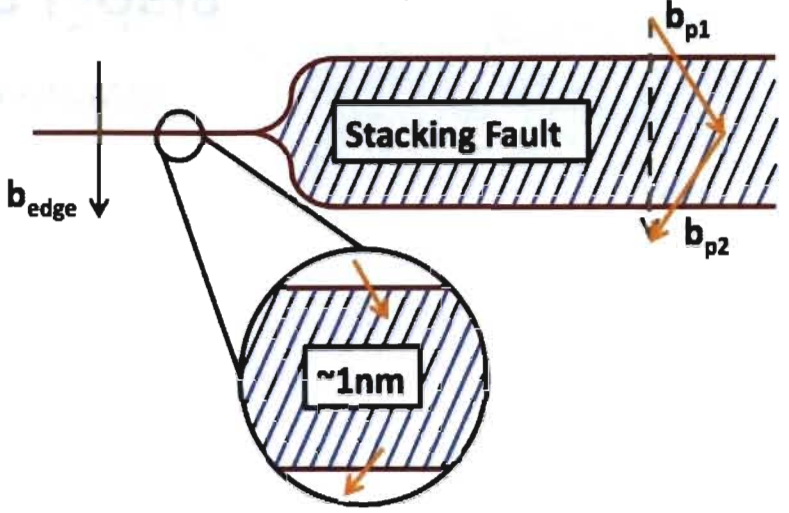
Vo, 2008

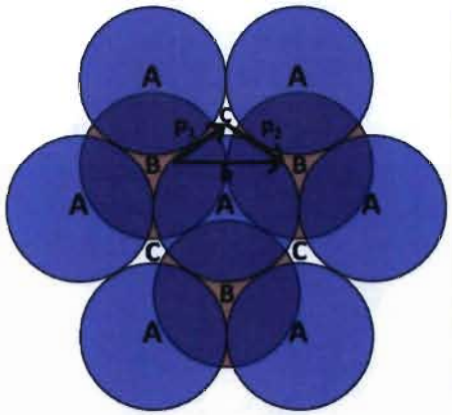
Van Swygenhoven, 1999; Yamakov, 2003; Wang, 2009; Chen, 2007

Partial Dislocations

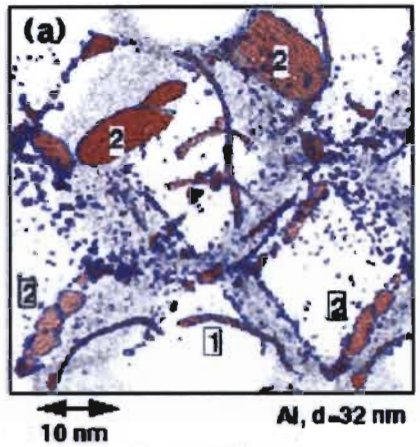
- fcc metals plastically deform through the motion of extended dislocations.
  - In bulk and large grained materials, these extended dislocations are very close (~1nm) and are often considered a single unit called a perfect dislocation.
  - In nanocrystalline metals, this assumption is inaccurate.
  - When atoms slide past each other they move in a zig-zag motion.
    - More energetically favorable.

Dissociation of a perfect edge dislocation.





Schematic showing slip and dislocation dissociation in a fcc metal.



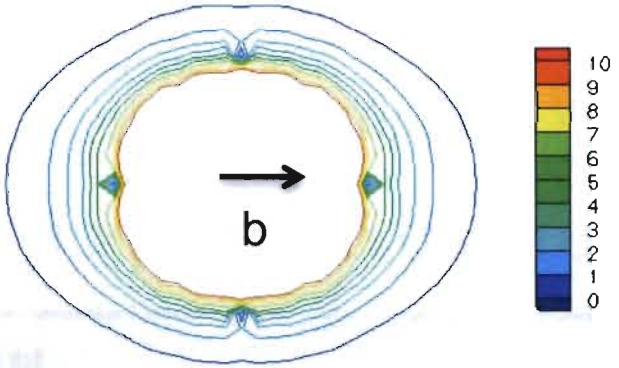
Yamakov, 2003

Outline

- 3D PFDD Model Formulation
  - Phase field variable
  - System energy and evolution
    - Elastic interaction energy
    - GSF Energy – Perfect Dislocations
    - GSF Energy – Partial Dislocations
      - Modeling the γ-surface
- Simulations and Results
  - Verification with analytical solution
  - Size Effects
    - Dislocation nucleation vs. dislocation growth
- Summary and Future Research Goals

Phase Field

- The phase field model tracks individual dislocations.
- The dislocation collective is described by the phase field variable, defined over each slip plane.
- Phase field is integer valued, and records (including sign) the number of dislocations that cross over the slip plane in units of the Burger's vector.
  - The location of a dislocation line corresponds to an integer jump in the phase field.

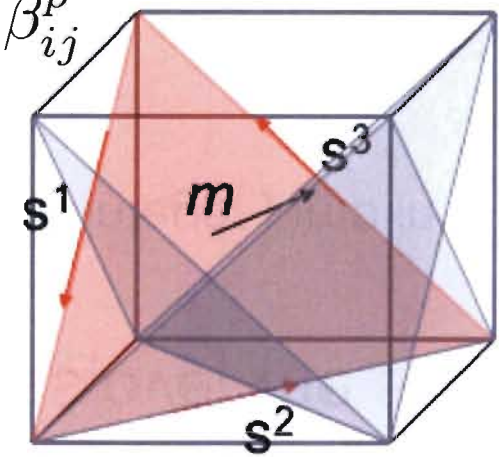


Hunter, 2009

Model Formulation

- Consider a crystal undergoing deformation
  - Elastic (reversible) deformation
  - Plastic (permanent) deformation

$$u_{i,j} = \beta_{ij}^{e} + \beta_{ij}^{p}$$



- Plastic deformation is mediated by the motion and interaction of dislocations
  - Can be directly related to the phase field:

$$\beta_{ij}^{p}(x) = \frac{1}{w}\sum_{\alpha=1}^{q} b(\alpha)\,\zeta(\alpha,x)\,s_i(\alpha)\,m_j(\alpha)$$

- Temporal evolution of the phase field is driven by minimization of the total energy of the system.

$$\frac{\partial \zeta(\alpha,x,t)}{\partial t} = -L\frac{\delta E}{\delta \zeta(\alpha,x,t)}$$

  - Steady-state Ginzburg-Landau Equation → $\dfrac{\delta E}{\delta \zeta(\alpha,x,t)} = 0$

Koslowski, 2002; Wang, 2001; Hunter, 2008

Dislocation Energy

- Total energy of the dislocation ensemble in a material system: $E = E^{elast} + E^{GSF}$
  - Elastic Interaction Energy
  - Core Energy
- Elastic Interaction Energy
  - Internal – dislocation-dislocation interactions
    - Elastic term, must be written in terms of the plastic phase field variable
  - External – dislocation interactions with applied stress
    - Zero applied stress for simulations presented later

$$E^{elast} = E^{int} + E^{ext} = \frac{1}{(2\pi)^3}\int\left[\frac{1}{2}C_{ijkl}\hat{\beta}^{p}_{mn}(k)\,\hat{\beta}^{p*}_{uv}(k) - k_i\hat{\sigma}_{ij}(k)\,\Omega_{jk}(k)\,\hat{\sigma}^{*}_{kl}(k)\,k_l\right]d^3k - \int \sigma^{appl}_{ij}\beta^{p}_{ij}d^3x$$

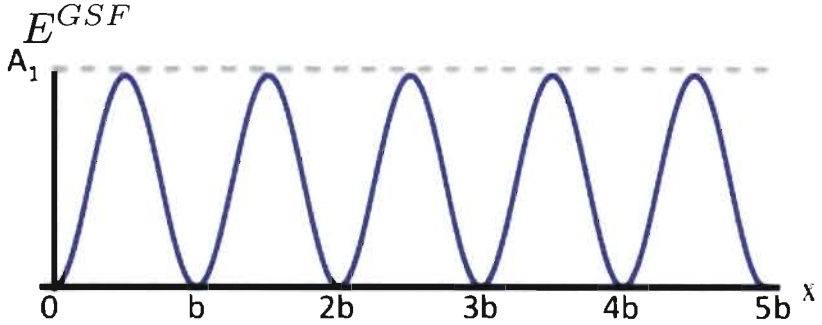
Koslowski, 2002; Wang, 2001; Hunter, 2008

GSF Energy – Perfect Dislocations

- Accounts for energy required to move the dislocation core through the crystal lattice
  - Mimics Peierls Potential
    - Periodic due to periodic nature of crystal lattice

$$E^{GSF} = \sum_{\alpha=1}^{3} \sum_{n=1}^{4} \int_{S_n} \phi_n^{\alpha}[\zeta_n^{\alpha}(x)] d^2x$$

- Can be described using several different functional forms
  - Piecewise Quadratic
  - Sinusoidal
    - Fourier Sine Series
      - Positive constant can be obtained from molecular dynamics (MD) simulations

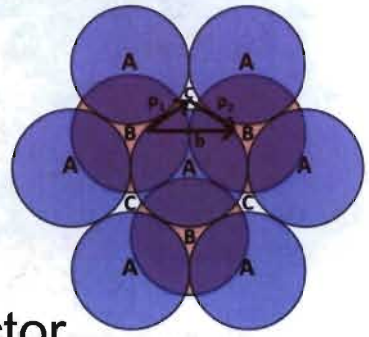


$$E^{GSF} = \int \left[\sum_{\alpha=1}^{q} A_1 sin^2(\pi \zeta(\alpha, x)) \right] d^3x$$

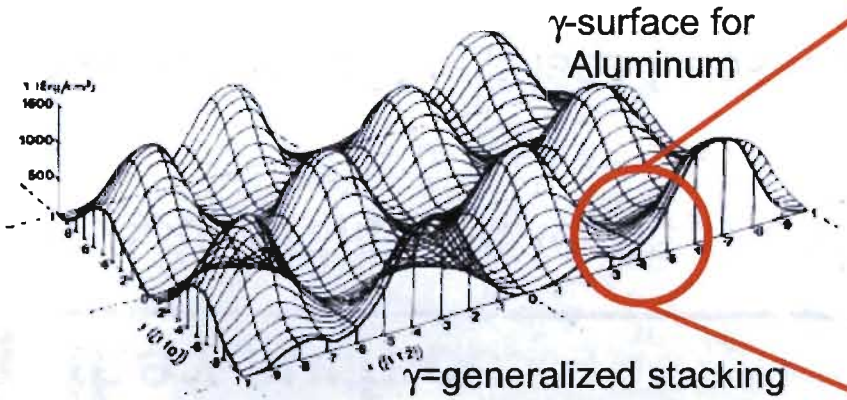
Koslowski, 2002; Ortiz, 1999; Wang, 2001; Hunter, 2010

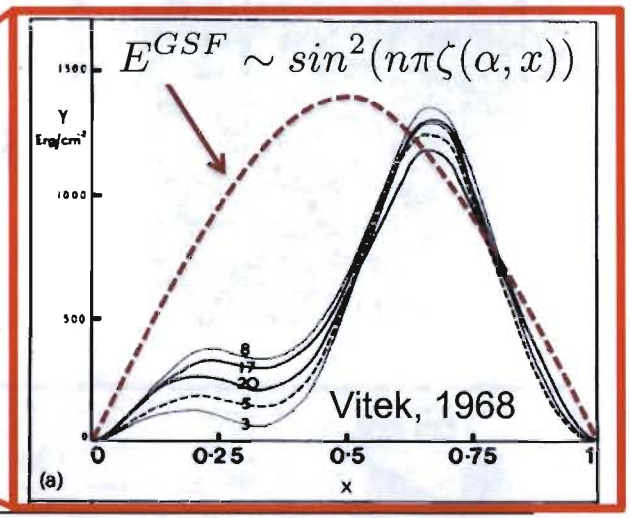
GSF Energy – Partial Dislocations

- Energetically favorable for defects to overcome two small energy barriers rather than one large barrier
  - Frank's rule ⟶ $b^2 > p_1^2 + p_2^2$
- γ-surface accounts for additional energy required to create a stacking fault
  - Global minima ⟶ displacement step of a Burger's vector
    - Lowest possible energy configuration
  - Local minima ⟶ partial dislocation direction



Hunter, 2011



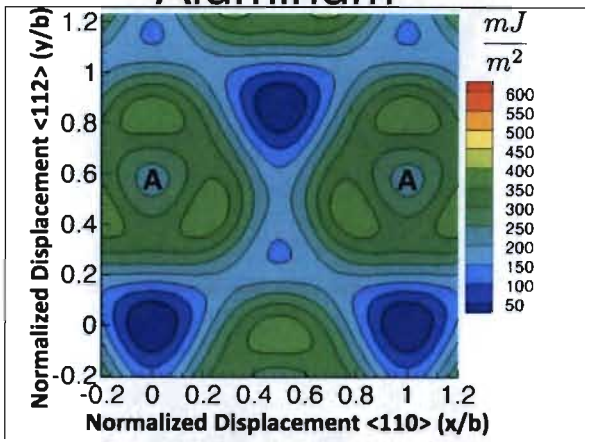


Modeling the γ-surface

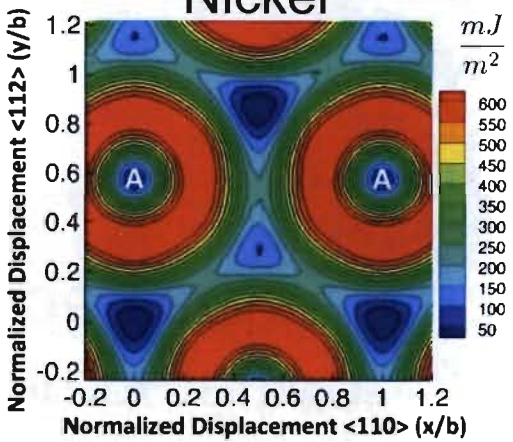
- The three active slip systems must be coupled
  - Linear combination of the phase fields needed to produce displacements in $\langle 112 \rangle$ directions
- Fit complex Fourier series to γ-surface found using MD simulations
  - 7 coefficients

$$
\begin{aligned}
E^{core}(\zeta_1,\zeta_2,\zeta_3) = \{ & c_0 + c_1[cos2\pi(\zeta_1-\zeta_2) + cos2\pi(\zeta_2-\zeta_3) + cos2\pi(\zeta_3-\zeta_1)] \\
& + c_2[cos2\pi(2\zeta_1-\zeta_2-\zeta_3) + cos2\pi(2\zeta_2-\zeta_3-\zeta_1) + cos2\pi(2\zeta_3-\zeta_1-\zeta_2)] \\
& + c_3[cos4\pi(\zeta_1-\zeta_2) + cos4\pi(\zeta_2-\zeta_3) + cos4\pi(\zeta_3-\zeta_1)] \\
& + c_4[cos4\pi(3\zeta_1-\zeta_2-2\zeta_3) + cos4\pi(3\zeta_1-2\zeta_2-\zeta_3) \\
& + cos4\pi(3\zeta_2-\zeta_3-2\zeta_1) + cos4\pi(3\zeta_2-2\zeta_3-\zeta_1) \\
& + cos4\pi(3\zeta_3-\zeta_1-2\zeta_2) + cos4\pi(3\zeta_3-2\zeta_1-\zeta_2)] \\
& + a_1[sin2\pi(\zeta_1-\zeta_2) + sin2\pi(\zeta_2-\zeta_3) + sin2\pi(\zeta_3-\zeta_1)] \\
& + a_3[sin4\pi(\zeta_1-\zeta_2) + sin4\pi(\zeta_2-\zeta_3) + sin4\pi(\zeta_3-\zeta_1)\}/w
\end{aligned}
$$

Aluminum



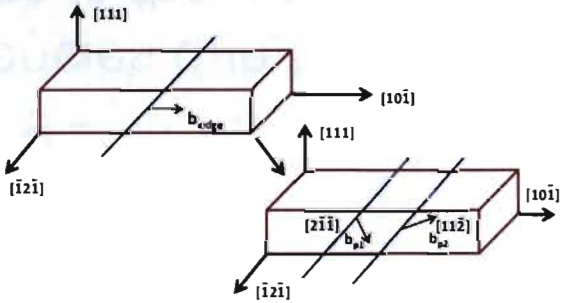
Nickel

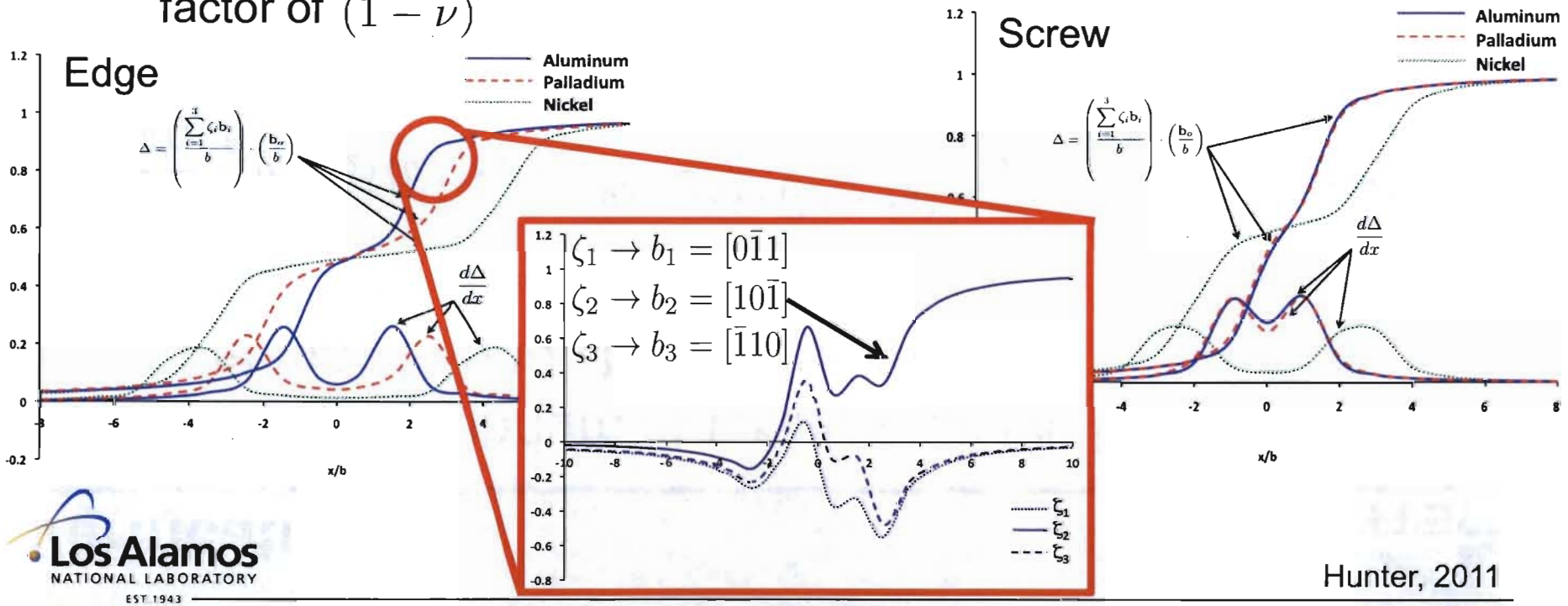


Vitek, 1968; Schoeck, 2001; Shen, 2004; Kim, 2010; Hunter, 2011

Simulations

- Infinitely long dislocation, periodic boundary conditions
  - Edge Orientation – Larger elastic energy component allows partials to dissociate farther
  - Screw Orientation – Elastic energy smaller by a factor of $(1-\nu)$





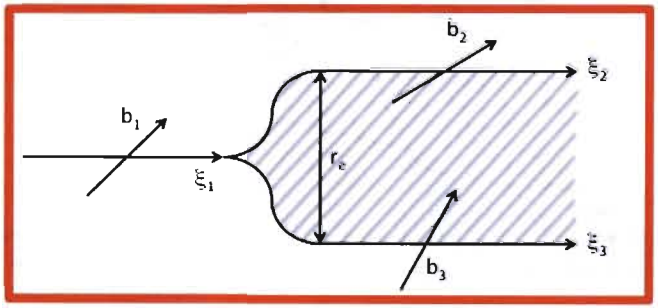
Hunter, 2011

Verification

- Compare equilibrium stacking fault widths from simulations to analytical solutions
  - Burger's vector reaction: $b_1 \rightarrow b_2 + b_3$ or $\frac{a}{2}[10\bar{1}] \rightarrow \frac{a}{6}[2\bar{1}\bar{1}] + \frac{a}{6}[11\bar{2}]$

$$\gamma_I = \frac{\mu}{2\pi r_e}\left[(b_2 \cdot \xi_2)(b_3 \cdot \xi_3) + \frac{(b_2 \times \xi_2)\cdot(b_3 \times \xi_3)}{1-\nu}\right]$$

Hirth and Lothe, 1982



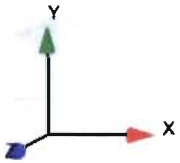
Material	Analytical (b)	Simulation (b)
Al^e	2.54	3.0 ± 0.5
Al^s	1.04	1.8 ± 0.5
Pd^e	4.15	4.9 ± 0.5
Pd^s	1.54	1.8 ± 0.5
Ni^e	8.04	8.1 ± 0.5
Ni^s	5.11	5.2 ± 0.5

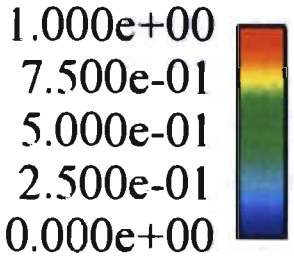
- Atomistics
  - Al^e: 2.8 – 13.3 b
  - Ni^e: 5.9 – 10.0 b
  - Ni^s: 2.9 – 10.1 b
- Discrepancies due to differences in the γ-surface from use of different atomic potentials

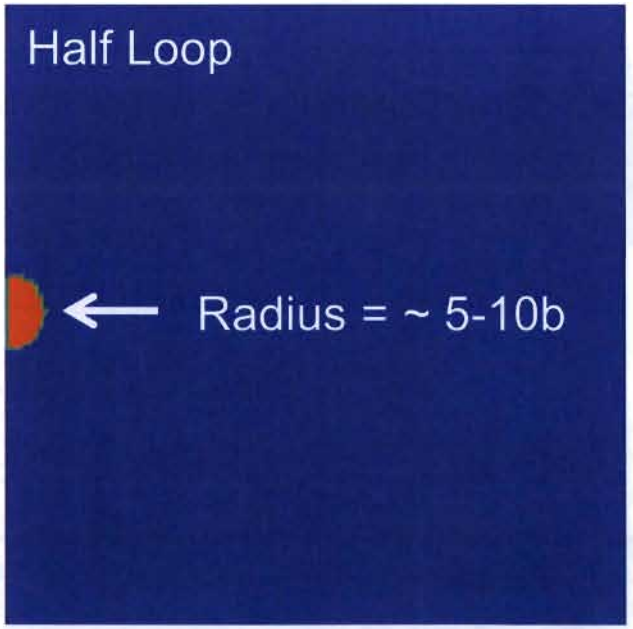
Hunter, 2011

Simulations

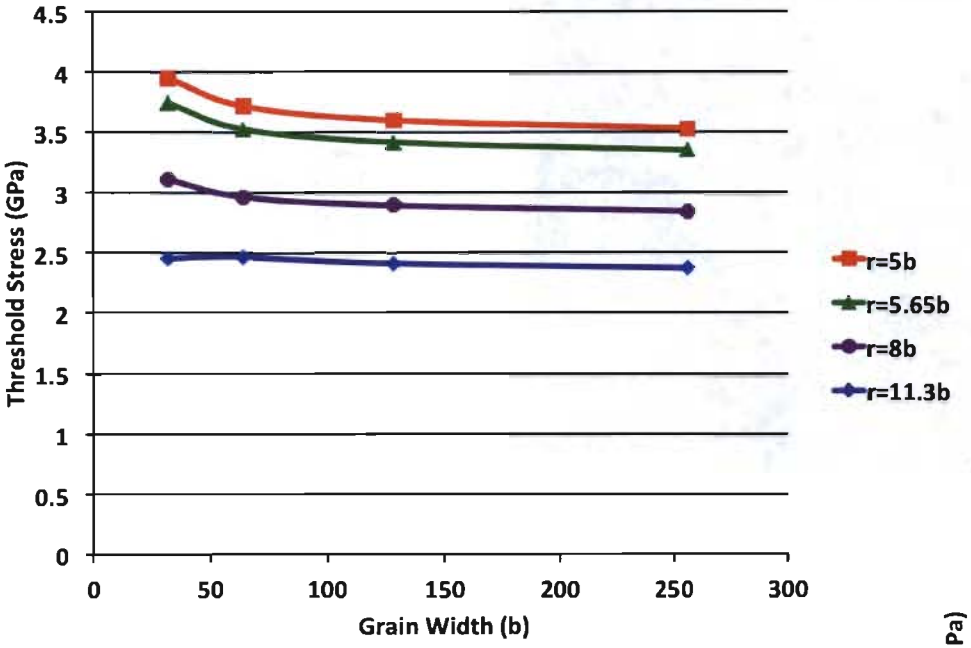
- Initial Conditions:
  - Perfect dislocation
    - Only 1 active phase field
  - Half Loop
  - Cluster of obstacles
    - Fixed/trapped dislocations
  - Nickel
- Boundary Conditions:
  - Fixed grain boundaries
    - 4b thick
- Applied Stress
  - Shear stress, σ_{13}





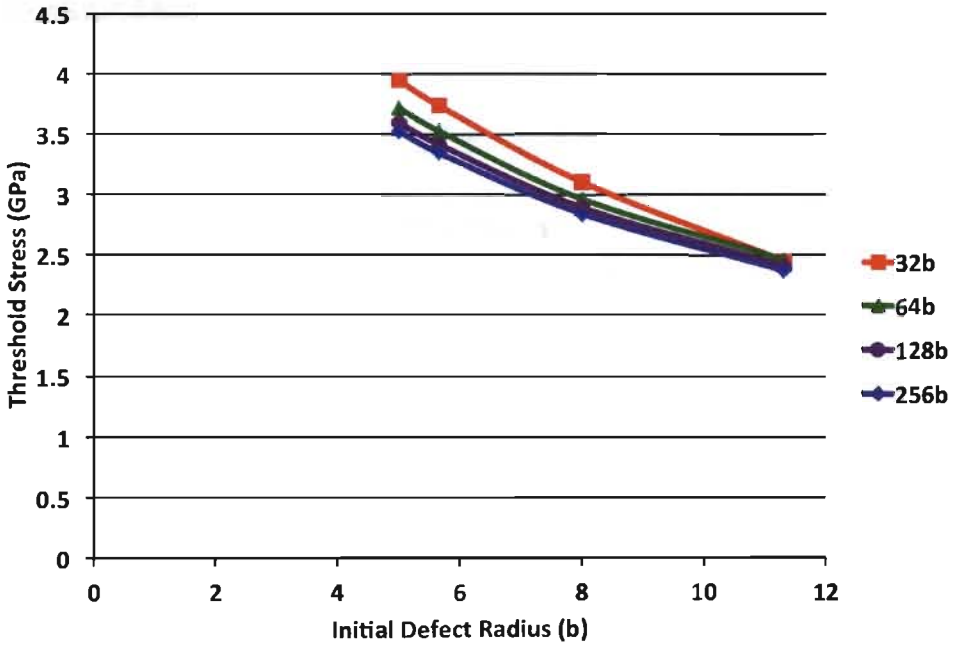


Dislocation Nucleation



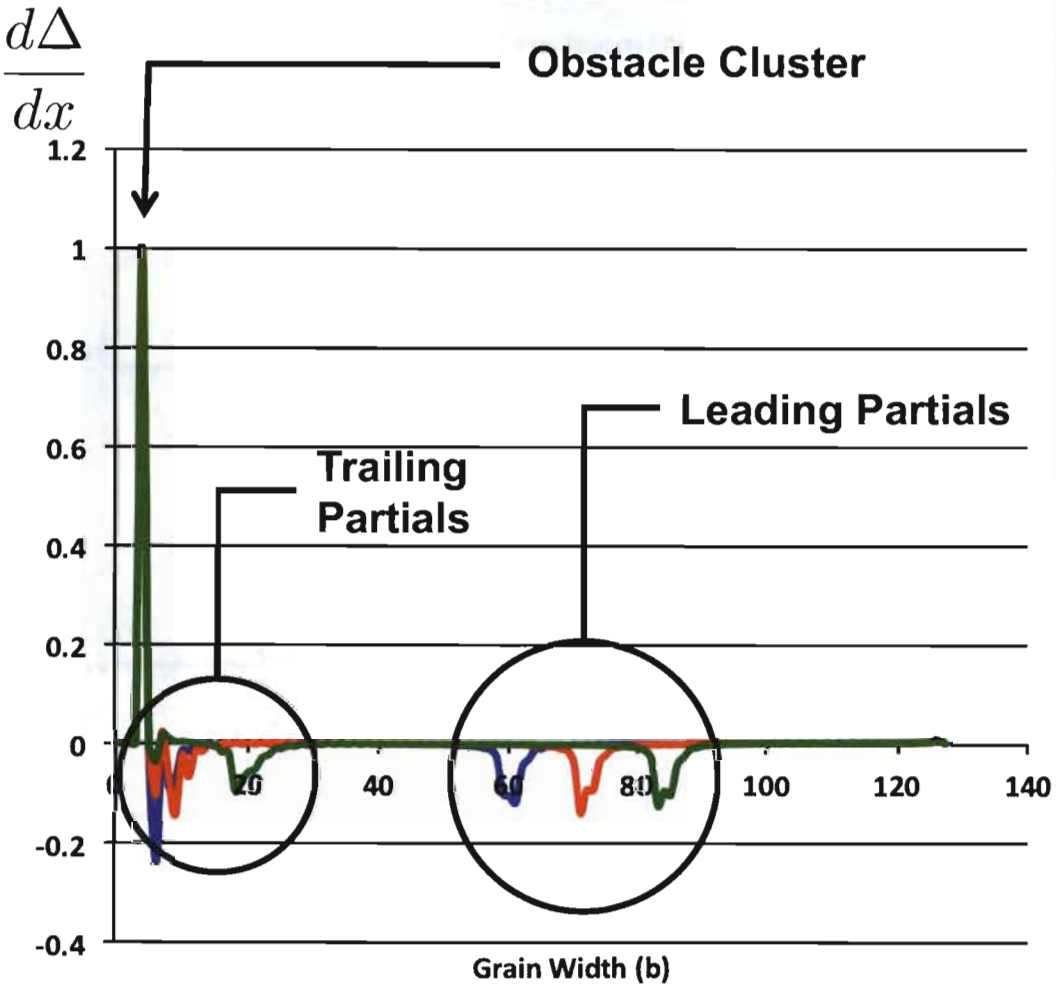
Grain size has little impact on defect nucleation

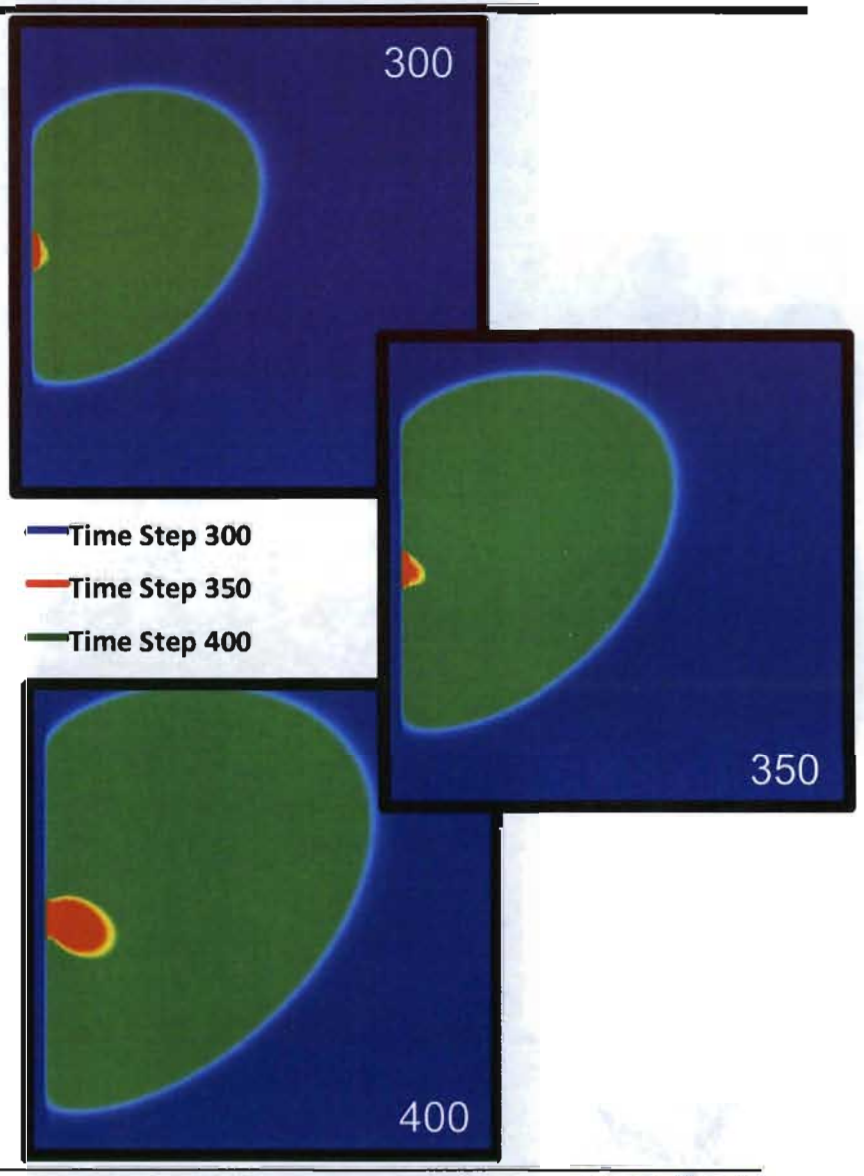
- Dependence seen in very small grain sizes
  - Dependence inversely proportional to initial defect size



- Defect nucleation is highly dependent on initial defect size

Dislocation Growth





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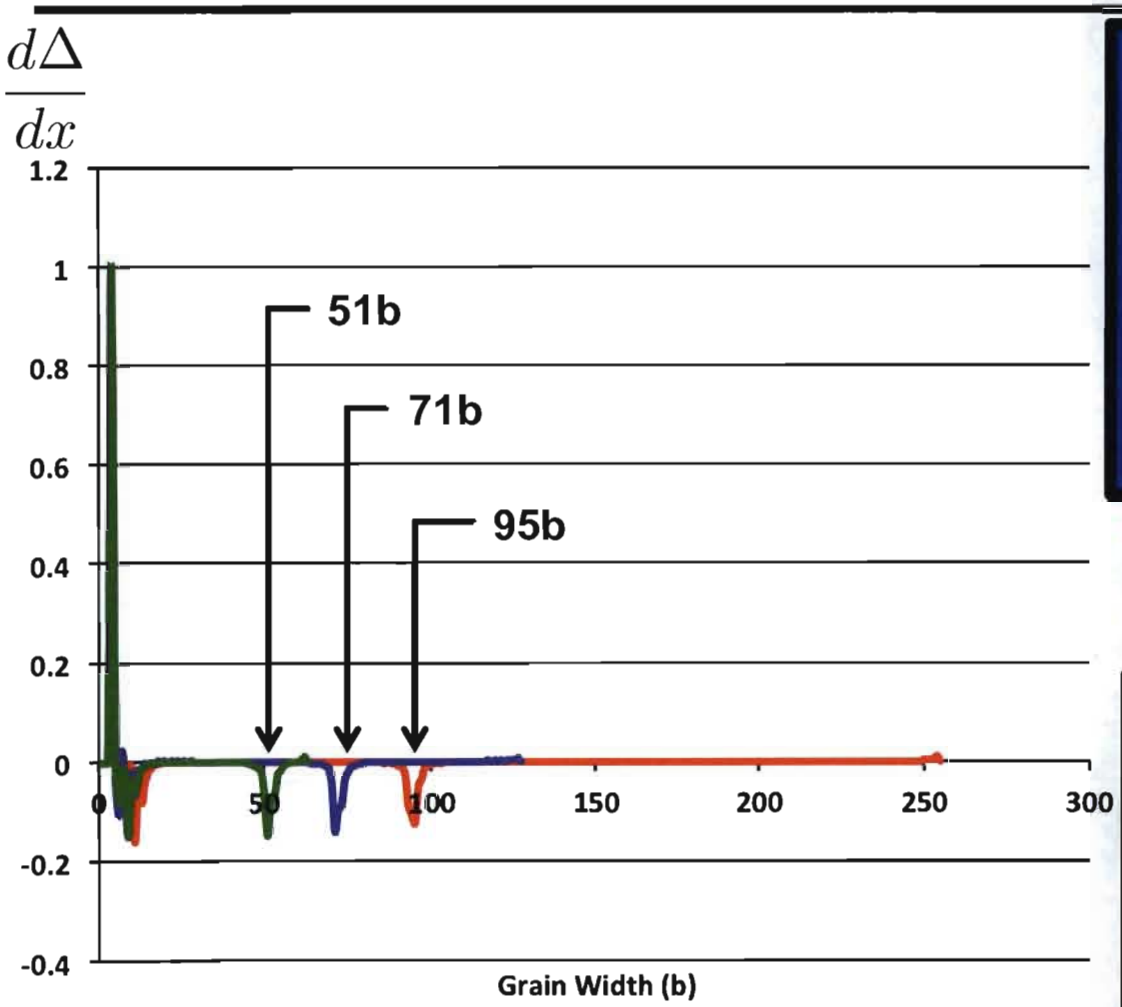
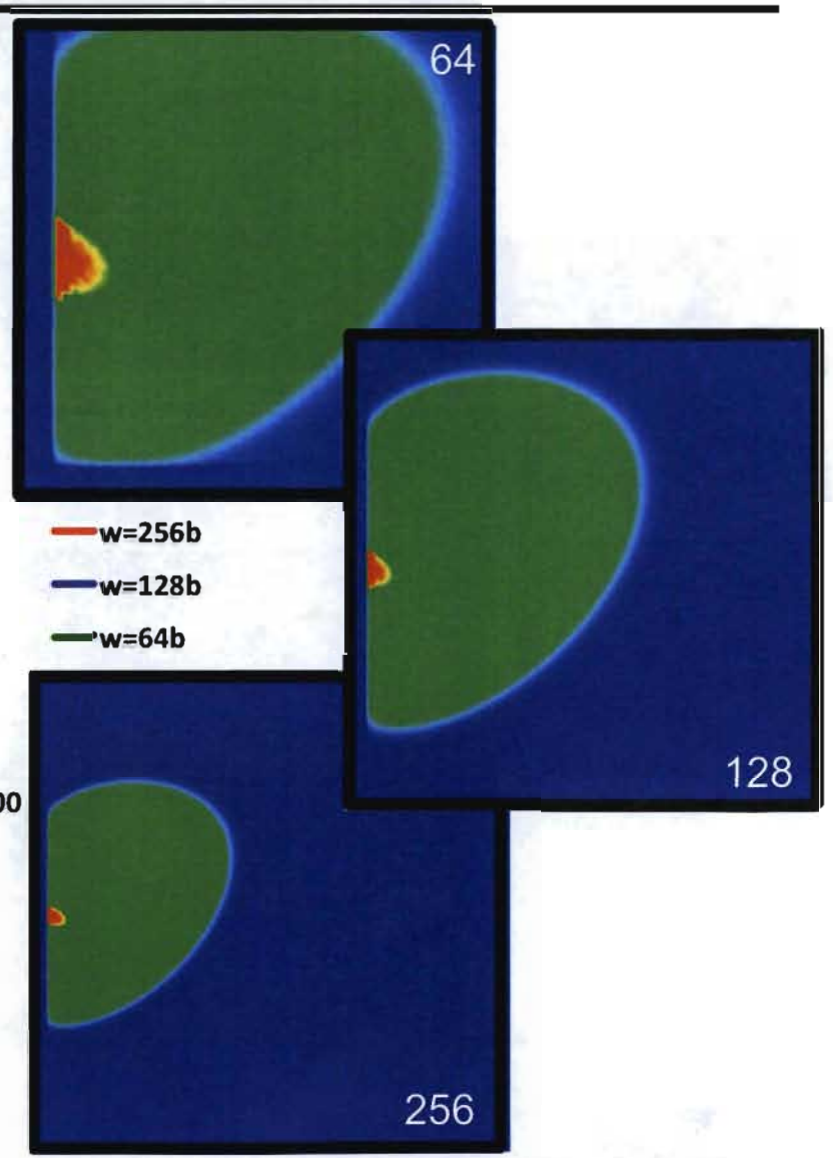
Size Effects





Summary and Future Research

- Successful implementation of partial dislocations through reformulation of the generalized stacking fault (GSF) energy
  - Included dependence of Peierls potential on the γ-surface
  - Results had good comparison to analytical solution and MD simulations
    - Infinitely long dislocation lines – equilibrium stacking fault widths
- Apply partial dislocation implementation to study size effects
  - Grain size variation has little impact on dislocation nucleation
    - Variation in the initial defect size has a much larger impact on nucleation
  - Grain Size variation does impact dislocation growth
    - Emergence of trailing partial has large dependence on grain size
- Future research goals
  - Investigate twinning
  - Implement grain boundary energy

References/Sponsers/Links

- Direct calculation of length scales in gradient plasticity theories, A. Hunter, M. Koslowski, **Journal Mechanics Physics Solids, 2008.**
- A continuum plasticity model that accounts for size effects and hardening in thin films, A. Hunter, H. Kavuri, M. Koslowski, **Modeling and Simulation in Materials Science and Engineering, 2010.**
- Large scale 3D phase field dislocation dynamics simulations on high performance architectures, Hunter, A., Saied, F., Le, C., and Koslowski, M., **International Journal of High Performance Computing Applications, 2010.**
- Influence of the stacking fault energy surface on extended partials in fcc metals with a 3D phase field dislocation dynamics model, A. Hunter, I.J. Beyerlein, T.C. Germann, M. Koslowski, **Physical Review B, 2011.**

- NNSA Center for Prediction of Reliability, Integrity and Survivability of Microsystems ASC-PSAAP

- Collaborators:
  - Marisol Koslowski (Purdue University)
  - Irene Beyerlein and Tim Germann (Los Alamos National Laboratory).
  - Hojin Kim and Alejandro Strachan (Purdue University)

http://www.purdue.edu/research/prism

October 2011

Abstract

The inelastic response of crystalline materials is mediated by dislocation motion and their interaction with defects, such as second phase particles, dislocations, grain boundaries and voids. Accounting for such defect interactions is particularly important when the scale of the volume analysis approaches low dimensional microstructure scales as in micron and sub-micron size devices, and nanocrystalline materials. Specifically, when the internal microstructure (i.e. grain size, film thickness) approaches tens of nanometers a transition in dominant deformation mechanisms occurs, and plasticity is mediated through the motion and interaction of Shockley partial dislocations in addition to perfect dislocations. This research investigates this deformation mechanism transition in fcc metals using a 3D phase field dislocation dynamics (3D PFDD) model that incorporates a dependency on the material γ-surface in order to model dislocation dissociation. In addition, size effects and the impact of confinement are discussed in relation to the stacking fault width between leading and trailing partial dislocations.